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Quantitative analysis of surface roughness evolution in FCC polycrystalline metal during uniaxial tension

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ABSTRACT

The purpose of this work is to present a quantitative description of surface roughness evolution in face-centered cubic (FCC) polycrystalline metal under uniaxial tension. The crystal plasticity model, in which the crystal plasticity constitutive law and the periodic boundary condition are incorporated, is established to analyze the effect of initial surface roughness, grain size and crystallographic orientation distribution on the surface roughness evolution. It is found that the surface topography during plastic straining can be divided into heterogeneous deformation surface and homogeneous deformation surface according to whether considering the heterogeneity of polycrystalline material or not. To quantitatively descript the surface roughness evolution during uniaxial tension, the concepts of equivalent grain size, which represents the comprehensive effect of grain sizes in different directions, and standard deviation of the direction cosines between crystal plane and rolling direction of grains (SD_cHR), which represents the effect of orientation distribution, are proposed. The roughness of the model with flat free surface depends approximately linearly on both the tension strain and the grain size, and exponential on the texture distribution. The uniaxial tensile test is performed to verify the accuracy of the established quantitative description of surface roughness evolution, which shows a favorable agreement with the predicted results.

1. Introduction

Surface roughening is an undesirable phenomenon in industrial practice. As a seemingly unavoidable phenomenon, surface roughening is commonly observed in plastically deformed polycrystalline metals. Surface roughness not only deteriorates the appearance of the product, but also influences other surface properties such as reflectivity, lubricant transport, weldability, adhesion and mechanical properties due to strain localization [1]. As a consequence, the surface roughening phenomenon has been extensively studied, including both experimental and numerical studies. It is commonly accepted that the surface roughness evolution during plastic process depends on the loading path, crystal structure, grain size, texture distribution, initial surface roughness of the product [2–4], etc. In those factors, the loading path and crystal structure are usually immutable in the production of specified products. However, the grain size, texture distribution and initial surface roughness can be easily changed in the pretreatment of materials (e.g. heat treatment).

Grain size is found to have a significant influence on surface roughening in some studies. Wouters et al. [5] investigated the surface roughening of polycrystalline Al–Mg alloys during tensile deformation. They observed a linear relation between root-mean-square roughness (S_q) and both strain and grain size. Similarly, Stoudt and Ricker [6] found that the roughening rate ($dR_a/d\varepsilon_{Pl}$) was dependent on the grain size in Al–Mg alloy, and the correlation between the roughening rate and grain size also appeared to be linear. Besides these research findings, some researchers had found deviations from the linear behavior. The work of Stoudt et al. [7] revealed that a linear relationship between S_q and plastic strain was more statistically appropriate for the finest grain size. As the grain size increased, the surface morphology became more complex and a quadratic model became more suitable.

Except for grain size, grain shape also affects the surface roughness after plastic deformation. Romanova et al. [1] had numerically studied the effects of the grain shape on surface roughening of aluminum alloys under uniaxial tension. They observed a pronounced surface roughness of equiaxial grain structure in comparison with that of extended grain structure.

Surface roughening originates in the heterogeneity of the polycrystalline material, whose grains have different crystal orientations leading to incompatibilities of deformation arising from the interactions between neighboring grains [8]. Stoudt et al. [9] found that a critical localization event was most likely to initiate in grain boundary regions where unfavorable slip interactions produced

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Nomenclature

cos(HKL, RD)	direction cosine between HKL and RD
cos(UVW, RD)	direction cosine between UVW and RD
$\bar{d}$	average grain size
d_e	equivalent grain size
HKL	crystal plane in Miller indices notation
ln(SD_M)	natural logarithm of SD_M
ln(SD_cHR)	natural logarithm of SD_cHR
ln(SD_cUR)	natural logarithm of SD_cUR
RD	rolling direction, i.e. the tensile direction in this paper
SD_cHR	standard deviation of cos(HKL, RD) in the model
SD_cUR	standard deviation of cos(UVW, RD) in the model
SD_M	standard deviation of Taylor factors in the model
S_q	root mean square deviation surface roughness
ΔS_q	surface roughness increasement
S_{q0}	initial surface roughness
S_{qd}	surface roughness of the differential surface topography
S_{qf}	final surface roughness of the model after stretching
S_{qf0}	final surface roughness of the no initial surface roughness model after stretching
UVW	crystal direction in Miller indices notation

the largest plastic strains. The impact of spatial distribution of crystallographic orientations and loading path were analyzed in the work of Liao and Chen [10]. The results showed that the surface roughness could be strongly related to the spatial distribution of microtexture and the sheet strained in the longitudinal direction displayed a dramatically smoother surface than that strained in the transverse direction.

Despite the basic understanding and qualitative analysis of the reasons inducing surface roughening, the effect of those factors, such as initial surface roughness and orientation distribution, on the surface roughness evolution are not yet comprehensively and quantitatively researched. In order to find out the quantitative relationship between surface roughening and both initial surface roughness, grain size and texture, the crystal plasticity model is adopted to simulate the surface roughness evolution of polycrystalline aluminum sheet during uniaxial tension process. And the accuracy of the quantitative description of surface roughness evolution is verified by the uniaxial tensile test.

2. Crystal plasticity finite element simulation procedures

2.1. Crystal plasticity theory

2.1.1. Kinematics

The rate-dependent constitutive relies on the multiplicative decomposition of the total deformation gradient (**F**), which is given by [11]:

$$\mathbf{F} = \mathbf{F}^* \cdot \mathbf{F}^{\mathbf{p}} \tag{1}$$

where $\mathbf{F}^{\mathbf{p}}$ denotes plastic shear of the material to an intermediate reference configuration in which lattice orientation and spacing are the same as in the original reference configuration, and $\mathbf{F}^*$ denotes stretching and rotation of the lattice. Elastic properties are assumed to be unaffected by slip, in the sense that stress is determined solely by $\mathbf{F}^*$. The rate of change of $\mathbf{F}^{\mathbf{P}}$ is related to the slipping rate $\dot{\gamma}^{(\alpha)}$ of the α slip system by:

$$\dot{\mathbf{F}}^{\mathbf{p}} \cdot \mathbf{F}^{\mathbf{p}^{-1}} = \sum_{\alpha} \dot{\gamma}^{(\alpha)} \mathbf{s}^{(\alpha)} \mathbf{m}^{(\alpha)} \tag{2}$$

where the sum ranges over all activated slip systems, unit vectors $\mathbf{s}^{(\alpha)}$ and $\mathbf{m}^{(\alpha)}$ are the slip direction and normal to slip plane in the reference configuration, respectively.

The slip direction vector $\mathbf{s}^{*(\alpha)}$ and the normal vector to the slip plane $\mathbf{m}^{*(\alpha)}$ in the deformed lattice are given by:

$$\begin{cases} \mathbf{s}^{*(\alpha)} = \mathbf{F}^* \cdot \mathbf{s}^{(\alpha)} \\ \mathbf{m}^{*(\alpha)} = \mathbf{m}^{(\alpha)} \cdot \mathbf{F}^{*^{-1}} \end{cases} \tag{3}$$

The velocity gradient in the current state is

$$\mathbf{L} = \dot{\mathbf{F}} \cdot \mathbf{F}^{-1} = \mathbf{D} + \mathbf{\Omega} \tag{4}$$

where the symmetric rate of stretching **D** and the antisymmetric spin tensor **Ω** may be decomposed into lattice parts and plastic parts as follows:

$$\mathbf{D} = \mathbf{D}^* + \mathbf{D}^{\mathbf{p}}, \quad \mathbf{\Omega} = \mathbf{\Omega}^* + \mathbf{\Omega}^{\mathbf{p}} \tag{5}$$

2.1.2. Constitutive laws and hardening of rate-dependent crystalline materials

The relation between the symmetric rate of stretching of the lattice, $\mathbf{D}^*$, and the Jaumann rate of Cauchy stress $\boldsymbol{\sigma}$, $\boldsymbol{\sigma}^{\nabla *}$, is given by [12]:

$$\boldsymbol{\sigma}^{\nabla *} + \boldsymbol{\sigma}(\mathbf{I} : \mathbf{D}^*) = \mathbf{L} : \mathbf{D}^* \tag{6}$$

where **I** is the second order identical tensor, and **L** is the 4 order tensor of elastic moduli.

Based on the Schmid law, the slipping rate $\dot{\gamma}^{(\alpha)}$ of the α slip system in a rate-dependent crystalline solid is determined by the corresponding resolved shear stress $\tau^{(\alpha)}$ as

$$\begin{cases} \dot{\gamma}^{(\alpha)} = \dot{\gamma}_0^{(\alpha)} \mathrm{sgn}(\tau^{(\alpha)}) |\tau^{(\alpha)}/\tau_c^{(\alpha)}|^n, & \text{for } \tau^{(\alpha)} \geqslant \tau_c^{(\alpha)} \\ \dot{\gamma}^{(\alpha)} = 0, & \text{for } \tau^{(\alpha)} < \tau_c^{(\alpha)} \end{cases} \tag{7}$$

where sgn(x) is the signum function, $\dot{\gamma}_0^{(\alpha)}$ is the reference value of the shear strain rate and n is the rate sensitive exponent. Both $\dot{\gamma}_0^{(\alpha)}$ and n are the material parameters. $\tau_c^{(\alpha)}$ is the critical resolved shear stress of the slip system α.

The strain hardening is characterized by the evolution of the strengths $\tau_c^{(\alpha)}$ through the incremental relation:

$$\dot{\tau}_c^{(\alpha)} = \sum_{\beta} h_{\alpha\beta} \dot{\gamma}^{(\beta)} \tag{8}$$

where $h_{\alpha\beta}$ are the slip hardening moduli, the sum ranges over all activated slip systems. Here $h_{\alpha\alpha}$ (no sum on α) and $h_{\alpha\beta}$ ($\alpha \neq \beta$) are called self and latent hardening moduli, separately. The self and latent hardening moduli are given by [13]:

$$h_{\alpha\alpha} = h_0 \mathrm{sech}^2 \left| \frac{h_0 \gamma}{\tau_s - \tau_0} \right|, \quad (\text{no sum on } \alpha) \tag{9}$$

$$h_{\beta\alpha} = q h_{\alpha\alpha}, \quad \beta \neq \alpha \tag{10}$$

where h_0 is the initial hardening modulus. τ_0 and τ_s are the yield stress and the breakthrough stress where large plastic flow initiates, respectively. γ is the Taylor cumulative shear strain on all slip systems. q is the latent hardening parameter. In this work, the AA6061 sheet is used for the numerical simulations and uniaxial tensile test. Fig. 1 shows both experimentally measured and numerically predicted stress-strain curves. Material parameters used for crystal